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TECHNICAL REPORT ARCCB-TR-95006

ADAPTIVE FINITE ELEMENT METHOD IV: MESH MOVEMENT

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FEBRUARY 1995

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (*Leave blank*)

2. REPORT DATE
February 1995

3. REPORT TYPE AND DATES COVERED
Final

4. TITLE AND SUBTITLE
ADAPTIVE FINITE ELEMENT METHOD IV:
MESH MOVEMENT

5. FUNDING NUMBERS
AMCMS: 6126.24.H191.1
PRON: 1A17Z1CBNMBJ

6. AUTHOR(S)
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
U.S. Army ARDEC
Benét Laboratories, AMSTA-AR-CCB-O
Watervliet, NY 12189-4050

8. PERFORMING ORGANIZATION REPORT NUMBER
ARCCB-TR-95006

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army ARDEC
Close Combat Armaments Center
Picatinny Arsenal, NJ 07806-5000

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

Accesion For

NTIS	CRA&I	X
DTIC	TAB	☐
Unannounced		☐
Justification		

By
Distribution /

Availability Codes

Dist	Avail and / or Special
A-1	

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

12b. DISTRIBUTION CODE

13. ABSTRACT (*Maximum 200 words*)

An adaptive finite element method is developed to solve initial boundary value problems for vector systems of parabolic partial differential equations in one space dimension and time. The differential equations are discretized in space using piecewise linear finite element approximations. Superconvergence properties and quadratic polynomials are used to derive a computationally inexpensive approximation to the spatial component of the error. This technique is coupled with time integration schemes of successively higher orders to obtain an approximation of the temporal and total discretization errors. The stability of several mesh equidistribution schemes for time-dependent partial differential equations is studied. The schemes move a finite difference or finite element mesh so that a given quantity is uniform over the domain. Mesh moving methods that are based on solving a system of ordinary differential equations for the mesh velocities are considered and some of these methods are shown to be unstable with respect to an equidistributing mesh when the partial differential system is dissipative. Simple criteria for determining the stability of a particular method are developed and the construction of stable differential systems for the mesh velocities is demonstrated. Several examples illustrating stable and unstable mesh motions are present.

14. SUBJECT TERMS
Parabolic Differential Equations, Adaptive Finite Elements, Equidistribution, Linear Stability, Mesh Movement

15. NUMBER OF PAGES
31

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std Z39-18
298-102

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INTRODUCTION

This is the fourth in a series of four reports whose overall purpose is to describe an adaptive finite element method (AFEM) for solving systems of parabolic partial differential equations. In particular, AFEM attempts to find a numerical solution of an M-dimensional system of the form

$$\boldsymbol{u}_t(x,t) + \boldsymbol{f}(x,t,\boldsymbol{u},\boldsymbol{u}_x) = [\boldsymbol{D}(x,t,\boldsymbol{u})\boldsymbol{u}_x(x,t)]_x \ , \ a<x<b \ , \ t>0 \ , \tag{1a}$$

subject to the initial conditions

$$\boldsymbol{u}(x,0) = \boldsymbol{u}^0(x) \ , \ a \le x \le b \tag{1b}$$

and linear separated boundary conditions

$$\begin{array}{l} \boldsymbol{A}^l(t)\boldsymbol{u}(a,t) + \boldsymbol{B}^l(t)\boldsymbol{u}_x(a,t) = \boldsymbol{g}^l(t) \\ \boldsymbol{A}^r(t)\boldsymbol{u}(b,t) + \boldsymbol{B}^r(t)\boldsymbol{u}_x(b,t) = \boldsymbol{g}^r(t) \end{array} , \ t>0 \ . \tag{1c}$$

The variables x and t represent spatial and temporal coordinates and denote partial differentiation when they are used as subscripts; $\boldsymbol{u}, \boldsymbol{f}, \boldsymbol{u}^0, \boldsymbol{g}^l$, and $\boldsymbol{g}^r$ are M-vectors; and $\boldsymbol{D}, \boldsymbol{A}^l, \boldsymbol{B}^l, \boldsymbol{A}^r$, and $\boldsymbol{B}^r$ are $M \times M$ matrices.

The problem is assumed to be well-posed and parabolic; thus, e.g., $\boldsymbol{D}(x,t,\boldsymbol{u})$ is positive definite. The rows of $\boldsymbol{B}^l$ and $\boldsymbol{B}^r$ are restricted to be either entirely zero or a row of the $M \times M$ identity matrix. When the i^{th} row of $\boldsymbol{B}^l$ or $\boldsymbol{B}^r$ is identically zero, then A^l_{ii} or A^r_{ii} cannot be zero, respectively, and the boundary condition is a Dirichlet (essential) condition. Otherwise, the boundary condition is a Neumann or Robbins (natural) condition. The ultimate goal of AFEM is to determine an approximate solution to Eq. (1) to within a user prescribed error tolerance.

The adaptive strategies utilized by AFEM are (1) error estimation coupled with (2) local mesh refinement (cf., e.g., Adjerid and Flaherty (ref 1), Babuska and Dorr (ref 2), Babuska, Zienkiewicz, Gago, and Oliveira (ref 3), Bank and Weiser (ref 4), Berger and Oliger (ref 5), Bieterman and Babuska (refs 6,7), Moore and Flaherty (ref 8), Shephard, Qingxiang, and Baehmann (ref 9), Strouboulis and Oden (ref 10), Zienkiewicz and Zhu (ref 11)), and (3) mesh movement (cf., e.g., Adjerid and Flaherty (ref 1), Arney and Flaherty (ref 12), Bell and Shubin (ref 13), Davis and Flaherty (ref 14), Dorfi and Drury (ref 15), Dwyer (ref 16), Ewing, Russell, and Wheeler (ref 17), Hyman (ref 18), Kansa, Morgan, and Morris (ref 19), Miller and Miller (refs 20,21), Petzold (ref 22), Rai and Anderson (ref 23), Russell and Ren (ref 24), Saltzman and Brackbill (ref 25), Smooke and Koszykowski (ref 26), Thompson (ref 27), Verwer, Blom, Furzeland, and Zegeling (ref 28), and White (ref 29)).

The purpose of this report is to describe the mesh moving procedures employed by AFEM. Detailed summaries of how AFEM implements its other adaptive strategies are found in separate reports entitled: Adaptive Finite Element Method II: Error Estimation (ref 30) and Adaptive Finite Element Method III: Mesh Refinement (ref 31). Furthermore, Adapative Finite Element Method I: Solution Algorithm and Computational Examples (ref 32) describes how all

the adaptive algorithms are implemented in unison and contains results demonstrating the utility of AFEM as a computational tool.

The mesh movement performed by AFEM is based on equidistribution. An *equidistributed mesh* is a partition of a spatial domain into elements such that a prescribed quantity is uniform over the mesh. More specifically, given an interval (a,b) and a positive weight function $w(x)$ defined on (a,b), then an equidistributed mesh is a partition

$$\Pi_N = \{a = x_0 < x_1 < x_2 < \ldots < x_{N-1} < x_N = b\} \tag{2a}$$

such that

$$\int_{x_{j-1}}^{x_j} w(x)dx = constant = \frac{1}{N}\int_a^b w(x)dx \quad , \quad j = 1,2,\ldots,N \, . \tag{2b}$$

Equidistribution has been used with functional approximation to determine the optimal placement of, e.g., interpolation points (cf., de Boor (ref 33) and Soanes (ref 34)). Equidistribution strategies have also been used in conjunction with the solution of two-point boundary value problems (cf., Pereyra and Sewell (ref 35)). The task of selecting a mesh to minimize the discretization error is known to be asymptotically equivalent to equidistributing the local discretization error when using the maximum norm (cf., de Boor (ref 33)).

Success with functional approximation and the numerical solution of ordinary differential equations has led investigators to consider the use of equidistribution strategies for generating moving meshes in conjunction with the numerical solution of transient partial differential equations (PDEs) (cf., Davis and Flaherty (ref 14)). The general framework is to simply reconsider Eq. (2) with a time dependency. Thus, the problem is to determine a dynamic mesh

$$\Pi_N(t) = \{a = x_0 < x_1(t) < x_2(t) < \ldots < x_{N-1}(t) < x_N = b\} \tag{3}$$

so that

$$\int_{x_{j-1}(t)}^{x_j(t)} w(x,t)dx = c(t) = \frac{1}{N}\int_a^b w(x,t)dx \, , \; j = 1,2,\ldots,N \, , \, t \geq 0 \, , \tag{4}$$

where $w(x,t) > 0, x \in [a,b], t \geq 0$, is usually chosen to be a function of the solution of the underlying PDE. For example, w has been chosen to be proportional to the solution's gradient, curvature, and local discretization error (cf., e.g., Adjerid and Flaherty (ref 1), Bell and Shubin (ref 13), Davis and Flaherty (ref 14), Dorfi and Drury (ref 15), Dwyer (ref 16), Rai and Anderson (ref 23), Russell and Ren (ref 24), Smooke and Koszykowski (ref 26), Verwer, Blom, Furzeland, and Zegeling (ref 28), and White (ref 29)).

When applying Eq. (4) in some numerical scheme, most investigators move a grid of a fixed number of elements to follow and resolve local nonuniformities in the solution. In order to guarantee accuracy, they must be sure that N, the number of elements, is large enough to approximate the solution throughout the entire spatial domain and the entire temporal integration. This is a relatively severe limitation since the optimal number of elements is not generally known in advance and generally varies with time.

Equidistribution techniques may be applied to time-dependent PDEs either by (1) solving Eq. (4) simultaneously with the solution of the PDEs; (2) extrapolating equidistributing meshes at past time levels to future time levels; or (3) integrating a system of ordinary differential equations for, say, the mesh velocities,

$$\frac{d}{dt}[x_j(t)] \doteq \dot{x}_j(t)\,,\; j = 0, 1, \ldots, N\,, \tag{5}$$

that are equivalent to Eq. (4). Many researchers have reported problems with extrapolating equidistributing meshes or with integrating differential equations for the mesh velocities. For example, if sufficient care is not exercised, mesh trajectories can leave the domain $[a,b]$, cross each other, or oscillate wildly from time step to time step. These events can even occur when the solution of the partial differential equations is changing very little.

Also, mesh moving is being used in conjunction with a numerical solution procedure for the PDEs. Since the accuracy of most PDE solution procedures depends on the uniformity of the space-time grid, equidistribution can deform the grid too much and introduce new and larger sources of discretization errors. As a result, some investigators have abandoned mesh moving in favor of local mesh refinement methods (cf., Berger and Oliger (ref 5) and Moore and Flaherty (ref 8)).

Refinement of a sufficient level can be used to guarantee that a solution has a prescribed accuracy; however, it is more costly than mesh motion since the solution must be recomputed. Additionally, refinement is less effective than mesh moving at reducing dispersive errors in the vicinity of wave fronts.

Our choice has been to combine local mesh refinement with mesh movement based on equidistribution. The benefits are twofold. First, refinement will avoid any drastic deformation of the grid caused by movement as well as guarantee a prescribed accuracy. Second, mesh movement will reduce the need for refinement and, thus, reduce computational costs.

In the following section, a method for solving the static equidistribution problem is discussed. Then in the Mesh Dynamics: Linear Stability section, static equidistribution is extended to a time-dependent partition, and a linear perturbation analysis is performed to examine its stability. In the Mesh Dynamics: Neutral Stability section, dynamic equidistribution is reformulated and its stability reexamined resulting in the construction of stable mesh moving schemes. Mesh Movement Implementation describes our numerical implementation of one of the stable mesh moving schemes constructed in Mesh Dynamics: Neutral Stability. Finally, in the last section, a summary of this report is presented.

STATIC SPATIAL EQUIDISTRIBUTION

The equidistribution problem Eq. (2) can most easily be solved by a technique due to de Boor (ref 33). Thus, we let

$$T(x,t) = \int_a^x w(\zeta,t)\,d\zeta \quad , \quad a \le x \le b \ . \tag{6}$$

Then

$$c(t) = \frac{1}{N}\,T(b,t) \tag{7}$$

and the equidistributing mesh $x_j(t)$, $j = 0,1,\ldots,N$, is determined as the solution of the nonlinear system

$$T(x_j(t),t) - jc(t) = 0 \ , \ j = 0,1,\ldots,N \ . \tag{8}$$

The equidistribution problem has a nonunique solution whenever $w(x,t) := 0$; hence, we may expect numerical difficulties when $w(x,t)$ is small on any subinterval of $[a,b]$. This problem is usually handled by imposing a lower bound on w, e.g., it is common to replace $w(x,t)$ by $w(x,t) + \eta$. There are many choices for the positive parameter η. Davis and Flaherty (ref 14) suggest that η should be related to the discretization error of the numerical method that is being used to solve the partial differential equations. Another popular choice (cf., e.g., Dwyer (ref 16)) is set to η to unity, when the interval $[a,b]$ and w have been appropriately scaled. Among other things, both of these choices ensure that the solution of Eq. (8) is a uniform mesh whenever w is small everywhere on $[a,b]$. Throughout the remainder of this report, we assume that $w(x,t) \ge 0$ for $a \le x \le b$, $t \ge 0$, with $w = 0$ only at a finite number of isolated points. This is sufficient to guarantee a unique solution of Eq. (8).

If $w(x,t)$ is a function of the numerical solution of the associated partial differential equations, it will generally only be known discretely. Suppose w is known at the points x_i^0, $i = 0,1,\ldots,M$, then we may approximate it by a piecewise polynomial in x and integrate Eq. (6) to find a piecewise polynomial approximation to $T(x,t)$. The function $c(t)$ can then be determined approximately from Eq. (7). An approximation x_j^1, $j = 0,1,\ldots,N$, to an equidistributing mesh is determined by solving Eq. (8) by, e.g., Newton iteration. If, in particular, we approximate $w(x,t)$ by a piecewise linear function of x with respect to the mesh x_i^0, $i = 0,1,\ldots,M$, then $T(x,t)$ is a piecewise quadratic function of x, and Eq. (8) can be solved for x_j^1, $j = 0,1,\ldots,N$, directly by the quadratic formula to give

$$x_j^1 = x_{i-1}^0 + \frac{2\gamma}{\beta + (\beta^2 + 2\alpha\gamma)^{1/2}} , \; j = 0,1,\ldots,N , \tag{9a}$$

where

$$\alpha = \frac{w(x_i^0,t) - w(x_{i-1}^0,t)}{x_i^0 - x_{i-1}^0} , \tag{9b}$$

$$\beta = w(x_{i-1}^0,t) , \; \gamma = jc - T(x_{i-1}^0,t) , \tag{9c,d}$$

and i is such that $T(x_{i-1}^0,t) \le jc \le T(x_i^0,t)$.

The number of points, M, in the input mesh x_i^0, $i = 0,1,\ldots,M$, and N, in the output mesh x_j^1, $j = 0,1,\ldots,N$, are not necessarily the same. This could be useful in situations where the function $w(x,t)$ is known very precisely, e.g., $w(x,0)$ can often be calculated exactly using the initial data of the associated partial differential equations. In this case, M can be determined so that the integrals in Eqs. (6) to (8) and the equidistributing mesh can be evaluated to a prescribed level of accuracy. For example, if the trapezoidal rule is used to approximate $T(x,t)$, an approximation of the equidistributing mesh $x_j(t)$, $j = 0,1,2,\ldots,N$, can be determined to tolerance ϵ by selecting

$$M^2 > \frac{(b-a)^3}{4\epsilon} \frac{\max_{a<x<b} w_{xx}(x,t)}{\min_{a<x<b} w(x,t)} \tag{10}$$

when $w(x,t) > 0$. This estimate is obtained from standard error formulae for the trapezoidal rule (cf., Dahlquist, Björk, and Anderson (ref 36)) and elementary continuity arguments.

When $N = M$, we may think of solving Eqs. (6) to (8) iteratively. Thus, the mesh x_j^1, $j = 0,1,\ldots,N$, can be used to calculate another approximation x_j^2, $j = 0,1,\ldots,N$, to an equidistributing mesh, etc. However, this iterative strategy does not necessarily converge near a local minimum of $w(x,t)$ as illustrated by the following simple example.

Example 1

Consider a three-point mesh ($M = N = 3$), x_j, $j = 0,1,2$, on $-1 \le x \le 1$ with $w(x,t) = x^2$. The endpoints $x_0 = -1$ and $x_2 = 1$ are fixed, and the only point that needs to be determined by iteration is x_1. The exact value of x_1 is, of course, zero; however, we start with an initial guess $x_1^0 = \epsilon$, use piecewise linear approximations for w, and see if successive iterates x_1^v, $v = 1,2,\ldots$, converge to zero. We can show that:

1. If $\epsilon = z := 2 - 3^{1/2}$, then $x_1^{2v+1} = -z$ and $x_1^{2v} = z$, $v = 0,1,....$ Thus, the iterative solution is a two-point limit cycle.

2. If $\epsilon \neq 0$, then, $|x_1^v| \leq z$, $v = 1,2,....$

3. If $|x_1^v| < z$, then $|x_1^v| < |x_1^{v+1}|$.

4. If $x_1^v > 0$, then $x_1^{v+1} < 0$.

Items (2) to (4) imply that x_1^v does not approach zero for any nonzero initial guess, but instead approaches a limit cycle, oscillating between z and $-z$ on alternate iterations.

The illustration of above items (1) to (4) is relatively simple. The piecewise linear approximation to $w(x,t) = x^2$ which interpolates to w at $x_1^0 = \epsilon$ is

$$f(x) = \begin{cases} 1 - (1 + x)(1 - \epsilon), & -1 \leq x \leq \epsilon \\ 1 - (1 - x)(1 + \epsilon), & \epsilon < x \leq 1 \end{cases} . \tag{11}$$

This implies that

$$T(\epsilon,t) = \frac{1}{2}(1 + \epsilon)(1 + \epsilon^2), \tag{12a}$$

$$T(1,t) = 1 + \epsilon^2, \tag{12b}$$

and

$$c(t) = \frac{1}{2}(1 + \epsilon^2). \tag{12c}$$

Now consider $\epsilon > 0$ (the case $\epsilon < 0$ follows from symmetry), then

$$T(0,t) = \frac{1}{2}(1 + \epsilon). \tag{13}$$

Since $0 < \epsilon < 1$, $c(t) < T(0,t)$, implying $x_1^1 < 0$. This proves item (4).

The solution x_1^1 is such that $T(x_1^1,t) = c(t)$, i.e.,

$$(1 + x_1^1) - \frac{1}{2}(1 + x_1^1)^2(1 - \epsilon) = \frac{1}{2}(1 + \epsilon^2). \tag{14}$$

This implies that

$$x_1^1 = \frac{\epsilon - \sqrt{1 - (1-\epsilon)(1+\epsilon^2)}}{1 - \epsilon}. \tag{15}$$

Now one might ask if there exists an ϵ such that $x_1^1 = -\epsilon$? The answer is found by substituting $-\epsilon$ for x_1^1 in Eq. (14). This substitution yields

$$(1 - \epsilon) - \frac{1}{2}(1 - \epsilon)^3 = \frac{1}{2}(1 + \epsilon^2). \tag{16a}$$

or

$$\epsilon - 4\epsilon^2 + \epsilon^3 = 0. \tag{16b}$$

Equation (16) factors into the following equation:

$$\epsilon[\epsilon - (2-\sqrt{3})][\epsilon - (2+\sqrt{3})] = 0. \tag{16c}$$

Since $z := 2 - 3^{1/2}$ is the only factor in the open interval (0,1), this result proves item (1).

Equation (16c) implies that if $0 < \epsilon < z$, then

$$\epsilon[\epsilon - (2-\sqrt{3})][\epsilon - (2+\sqrt{3})] > 0. \tag{17}$$

Equation (17) implies that $T(-\epsilon,t) > c(t)$. Therefore, $x_1^1 < -\epsilon$ whenever $0 < \epsilon < z$. This proves item (3).

All that remains is to prove item (2). Rewrite ϵ as $z + \epsilon_z$, where ϵ_z is such that $-1 < z + \epsilon_z < 1$. Then item (2) is true if $T(-z,t) < c(t)$. This implies that item (2) is true if

$$(1 - z) - \frac{1}{2}(1 - z)^2(1 - (z-\epsilon_z)) < \frac{1}{2}(1 + (z+\epsilon_z)^2). \tag{18}$$

Equation (18) reduces to

$$\frac{1}{2}(1 - 2z + z^2)\epsilon_z < \frac{1}{2}(2z\epsilon_z + \epsilon_z^2) \tag{19a}$$

or

$$0 < -\frac{1}{2}(1 - 4z + z^2)\epsilon_z + \frac{1}{2}\epsilon_z^2. \tag{19b}$$

Since z is a root of the quadratic term of Eq. (19b), this implies that item (2) is true if

$$0 < \frac{1}{2}\epsilon_z^2 . \tag{20}$$

This proves item (2).

MESH DYNAMICS: LINEAR STABILITY

The discussion of the previous section involved the computation of an equidistributing mesh at one time. As noted in the Introduction, equidistributing meshes at subsequent time levels can be obtained by a variety of techniques. In this section, we use linear stability analyses to explain why many researchers have been experiencing difficulties when using either extrapolation or ordinary differential equations for mesh velocities to obtain equidistributing meshes. There are no stability problems associated with solving Eq. (8) directly; however an objection to this approach is the complexity associated with solving differential-algebraic systems for the partial differential equation solution and the mesh motion.

We begin our analysis by considering a system obtained by differentiating Eq. (8) with respect to time. Upon use of Eq. (6), this gives

$$w(x_j,t)\dot{x}_j = -\left[\int_a^{x_j} w_t(x,t)dx - j\dot{c}(t)\right], \; j = 1,2,\ldots,N-1 . \tag{21}$$

Suppose $x_j(t)$, $j = 0,1,\ldots,N$, is an equidistributing mesh that exactly satisfies Eqs. (8) and (21) for $t \geq 0$. Let us introduce a small perturbation $\delta x_j(0)$, $j = 0,1,\ldots,N$, at $t = 0$ and study its effect on Eq. (21). If no additional errors are introduced, the perturbed system satisfies

$$w(x_j(t)+\delta x_j(t),t)\,(\dot{x}_j+\delta\dot{x}_j) = -\left[\int_a^{x_j+\delta x_j} w_t(x,t)dx - j\dot{c}(t)\right], \quad j = 1,2,\ldots,N-1 , \tag{22}$$

subject to the constraints $\delta x_0(t) = \delta x_N(t) = 0$. We further assume that $|\delta x_j| << b - a$, $j = 1,2,\ldots,N-1$, and linearize Eq. (22) to get

$$\frac{d}{dt}[w(x_j(t),t)\delta x_j(t)] = 0 , \; j = 1,2,\ldots,N-1 . \tag{23}$$

Integrating, we find

$$\delta x_j(t) = \frac{w(x_j(0),0)}{w(x_j(t),t)}\delta x_j(0) , \; j = 1,2,\ldots,N-1 . \tag{24}$$

Therefore, the differential system Eq. (21) is stable to linear perturbations if is less than unity. Unfortunately, most choices of $w(x,t)$ are likely to be decaying functions of time for dissipative parabolic systems, and this will almost certainly yield a value of $L(t)$ that is

$$L(t) = \max_{0<j<N} \frac{w(x_j(0),0)}{w(x_j(t),t)} \tag{25}$$

larger than unity. Local instabilities can also occur whenever the mesh is moved so that $L(t)$ exceeds unity for some specific times. These instabilities may grow or decay as time progresses depending on the value of L.

The following two examples illustrate some of the instabilities that can occur.

Example 2

Consider the heat conduction problem

$$u_t = \frac{1}{\pi^2} u_{xx} \ , \ 0 < x < 1 \ , \ t > 0 \ , \tag{26a}$$

$$u(x,0) = \sin \pi x \ , \ u(0,t) = u(1,t) = 0 \ . \tag{26b,c}$$

The exact solution of this problem is

$$u(x,t) = e^{-t} \sin \pi x \ . \tag{26d}$$

We take

$$w(x,t) \propto |u_{xx}(x,t)| \ . \tag{26e}$$

Since $u(x,t)$ and $w(x,t)$ are separable in space and time, the correct strategy is to generate an equidistributed mesh at time $t = 0$ and use it for all time. However, $L(t) \propto \exp(-t)$, and thus we expect the solution of Eq. (21) to be unstable. In Figure 1 (at the end of this section), we display the meshes produced by both Eqs. (8) (dashed curves) and (21) (solid curves), and the unstable behavior of Eq. (21) is clearly visible. Simpson's rule with $M = 200$ was used to evaluate all integrals, a mesh of $N = 10$ elements was equidistributed, and an initial perturbation $\delta x_j(0) = 0.025, j = 1,2,...,N-1,$ was introduced. Equations (21) (and all differential equations appearing in Example 3) were solved using a version of the differential-algebraic equation solver DASSL (cf., Petzold (ref 37)).

Example 3

We consider a problem for a partial differential equation that has the exact solution

$$u(x,t) = \tanh r_1[(x-1) + r_2 t] \ , \ 0 \le x \le 1 \ , \ t \ge 0 \ . \tag{27}$$

The function (27) is a wave that travels in the negative x direction when r_1 and r_2 are positive (cf., Figure 2 at the end of this section). The values of r_1 and r_2 determine the steepness of the wave

and its propagation speed. Such solutions could arise from several types of partial differential equations, e.g., Davis and Flaherty (ref 14) studied a heat conduction problem of the form

$$u_t + f(x,t) = \frac{1}{\sigma^2} u_{xx} \ , \ 0 \leq x \leq 1 \ , \ t > 0 \ , \tag{28}$$

where the initial conditions, Dirichlet boundary conditions, constant diffusion σ^{-2}, and source f were chosen so that the exact solution was given by Eq. (27).

The meshes produced by both Eqs. (8) (dashed curves) and (21) (solid curves) for $r_1 = 5$, $r_2 = 1$ and

$$w(x,t) \propto |u_x(x,t)| + \eta \ , \tag{29}$$

where $\eta = 0.1$, are shown in Figure 3 (at the end of this section). The solution of Eq. (21) is marginally stable for small times, but w decreases as the wave front progresses towards $x = 0$, and the instability is apparent. In fact, some mesh trajectories have left the domain [0,1]. Simpson's rule with $M = 200$ was used to evaluate all integrals, a mesh of $N = 10$ elements was equidistributed, and an initial perturbation $\delta x_j(0) = 0.025, j = 1,2,...,N\text{-}1$, was introduced.

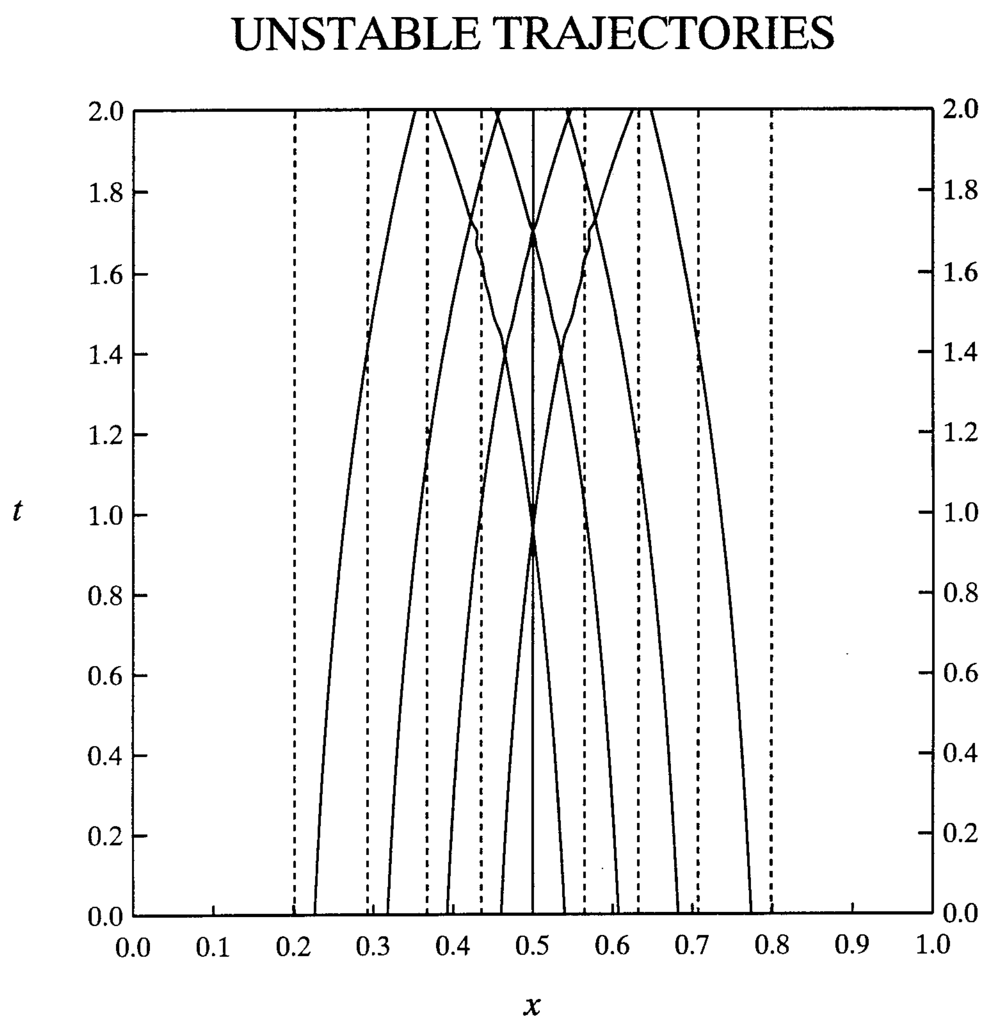

Figure 1. Mesh trajectories for Example 2.

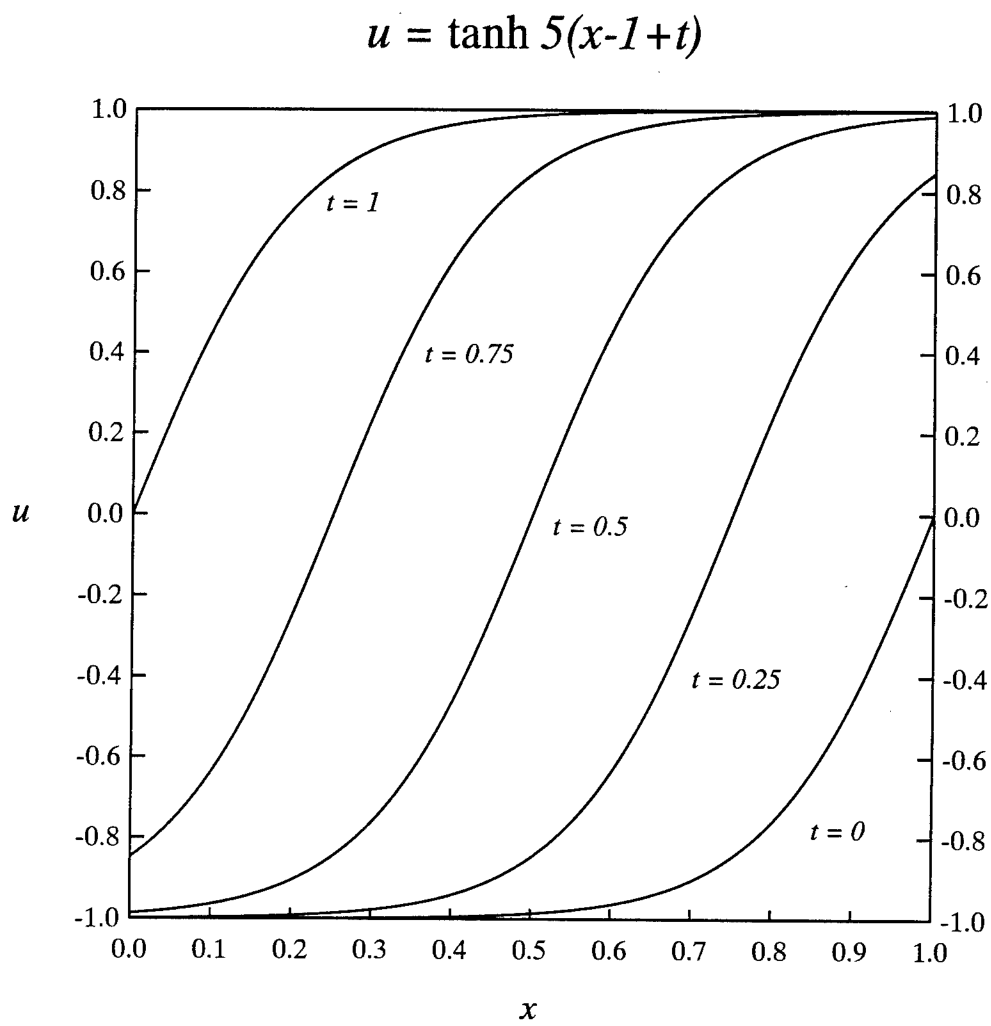

Figure 2. Graphs of Eq. (27) for selected instances of time.

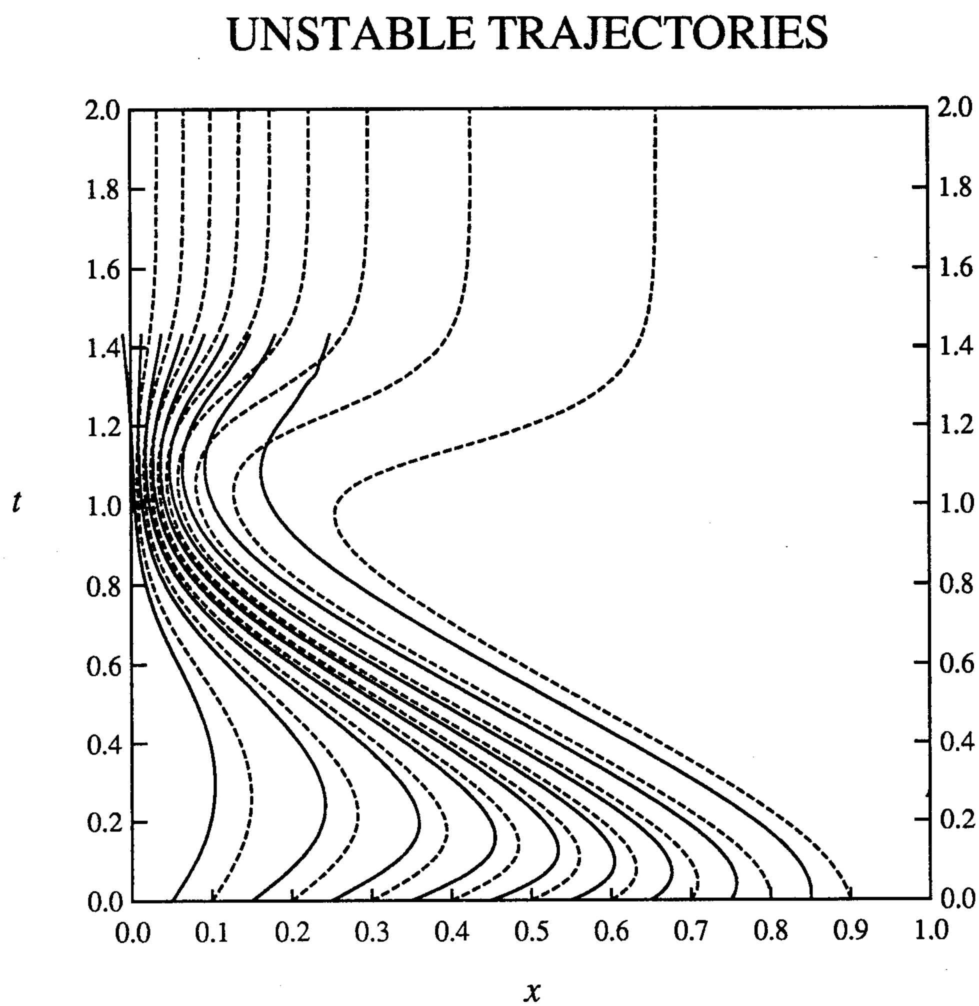

Figure 3. Mesh trajectories for Example 3.

MESH DYNAMICS: NEUTRAL STABILITY

In the previous section, it was shown how in certain instances mesh moving could become unstable. Such instabilities help to explain the oscillations that some researchers have observed with mesh movement. However, other researchers have seen no such instabilities develop in their mesh moving schemes, even when solving dissipative problems. The results of the previous section do not give sufficient guidance to support the construction of stable mesh moving schemes. In order to explore this further and to more fully understand the dynamics of mesh movement, define

$$\Phi(x,t) \doteq \frac{T(x,t)}{T(b,t)} = \frac{\int_a^x w(\zeta,t)d\zeta}{\int_a^b w(\zeta,t)d\zeta} \tag{30}$$

(cf., Eq. (6)) and rewrite Eq. (8) as

$$\Phi(x_j(t),t) - \frac{j}{N} = 0 \; , \; j = 0,1,...,N \; . \tag{31}$$

Now consider the differential system,

$$\frac{d}{dt}[\Phi(x_j(t),t)] = 0 \; , \; j = 1,2,...,N-1 \tag{32}$$

obtained by differentiating Eq. (31) with respect to time.

The next step is to perform the same stability analysis on Eq. (32) as was done on Eq. (21) in the previous section. This perturbation analysis can be simplified by noting that Eq. (31) is identical to Eq. (8) with the weight function $w(x,t)$ replaced by the normalized weight function

$$W(x,t) = \frac{w(x,t)}{\int_a^b w(\zeta,t)d\zeta} \tag{33}$$

Recall that $w(x,t)$ is zero at only a finite number of isolated points; hence, $W(x,t)$ is well defined. Therefore, the result of the stability analysis for Eq. (32) can be found by replacing w by W in Eq. (25). The differential system Eq. (32) is stable to linear perturbation, then, if

$$\bar{L}(t) = \max_{0<j<N} \frac{W(x_j(0),0)}{W(x_j(t),t)} \tag{34}$$

is less than unity.

At first glance, it would appear that the stability determination has simply shifted from $w(x,t)$ to $W(x,t)$; thus, instability occurs when $\bar{L}(t) > 1$ or when $W(x_j(t),t)$ is a decreasing function of time. However, if Eq. (34) is rewritten with Eq. (33) used to indicate the dependence of $w(x,t)$, the result is

$$\bar{L}(t) = \max_{0<j<N} \frac{w(x_j(0),0)}{w(x_j(t),t)} \frac{\int_a^b w(\zeta,t)d\zeta}{\int_a^b w(\zeta,0)d\zeta} . \tag{35}$$

The conditions expressed by Eq. (35) are potentially less severe than those of Eq. (25) since

$$\bar{L}(t) \le L(t) \tag{36}$$

whenever $w(x,t)$ is a decreasing function in time. Some improvement may have occurred, although there is still no guarantee of stability. Significant improvement does occur when $w(x,t)$ is a separable function of space and time (cf., Example 2). In this case, $\bar{L}(t) = 1$; thus, mesh motion is neutrally stable whether $w(x,t)$ is decreasing or not. Thus, for any separable function $w(x,t)$, small perturbations of Eq. (32) will not grow or decay as time increases.

Example 4

Reconsider Example 2 where $w(x,t)$ was given by Eq. (26). Recall that Eq. (21) generated unstable mesh motion because $L(t) \propto \exp(-t)$. Since $\bar{L}(t) = 1$ for this function $w(x,t)$, the solution of Eq. (32) should show no evidence of these instabilities. In Figure 4 (at the end of this section) meshes produced by both Eqs. (31) (dashed curves) and (32) (solid curves) are displayed. As predicted, mesh trajectories generated by Eq. (32) remain neutrally stable for all time. As in Example 2, Simpson's rule with $M = 200$ was used to evaluate all integrals, a mesh of $N = 10$ elements was equidistributed, and an initial perturbation of $\delta x_j(0) = 0.025, j = 1,...,10,$ was introduced. Equation (32) was solved using a version of the differential-algebraic solver, DASSL (cf., Petzold (ref 37)).

Equidistribution through Eq. (32) does not guarantee that initial small perturbations do not grow unless $w(x,t)$ is separable. However, if Eq. (32) is reexamined, with emphasis placed on the stability of the functions $\Phi(x_j(t),t), j = 1,...,N-1,$ the results are different. In order to see this, define

$$\Phi_j(t) = \Phi(x_j(t),t) \ , \ j = 0,1,...,N \tag{37}$$

and rewrite Eq. (32) as

$$\frac{d}{dt}[\Phi_j(t)] = 0 \ , \ j = 1,2,...,N-1 \ . \tag{38}$$

The stability results are obvious in terms of these new dependent variables. Equation (38) is neutrally stable and initial perturbations of Φ_j (through x_j), $j = 1,...,N-1$ will neither grow nor decay. This does not imply that the mesh trajectories are neutrally stable. However, a type of

stability is inherited. If $\delta x_j(0)$, $j = 1,2,...,N\text{-}1$, is such that

$$x_{j-1}(0) < x_j(0) + \delta x_j(0) < x_{j+1}(0) \ , \ j = 1,2,...,N-1 \ , \tag{39a}$$

then solutions of Eq. (33) will ensure that

$$x_{j-1}(t) < x_j(t) + \delta x_j(t) < x_{j+1}(t) \ , \ j = 1,2,...,N-1 \ , \tag{39b}$$

for all $t > 0$.

Example 5

Reconsider Example 3 where $w(x,t)$ was given by Eq. (29). Recall that Eq. (21) generated unstable mesh motion because w decreased as the wave front progressed to $x = 0$. Solutions of Eq. (38) should demonstrate no such instabilities. In Figure 5 (at the end of this section) meshes produced by both Eqs. (31) (dashed curves) and (38) (solid curves) are displayed. As predicted, mesh trajectories generated by Eq. (38) remain bounded for all time and do not intersect. As in Example 4, Simpson's rule with $M = 200$ was used to evaluate all integrals, a mesh of $N = 10$ elements was equidistributed, and an initial perturbation of $\delta x_j(0) = 0.025$, $j = 1,2,...,10$, was introduced. Equation (38) was solved using a version of the differential-algebraic solver, DASSL (cf., Petzold (ref 37)).

Furthermore, if Eq. (21) is rewritten in terms of Φ_j, $j = 1,2,...,N\text{-}1$, the result is

$$\frac{d}{dt}[\Phi_j(t)] + \lambda(t)\Phi_j(t) = \frac{j}{N}\lambda(t) \ , \ j = 1,2,...,N-1 \ , \tag{40a}$$

where

$$\lambda(t) = \frac{\int_a^b w_t(\zeta,t)d\zeta}{\int_a^b w(\zeta,t)d\zeta} \ . \tag{40b}$$

Equation (40) will be asymptotically stable if $\lambda(t) > 1$ and neutrally stable when $\lambda(t) = 1$. Initial perturbations will grow when $\lambda(t) < 1$. The condition, $\lambda(t) < 1$, will occur when $w_t(x,t) < 0$, i.e., when $w(x,t)$ is a decreasing function of time. This result is stronger than that of the previous section, since arbitrary perturbations are permitted.

Equation (40) also demonstrates how to form asymptotically stable mesh moving equations, if so desired. Simply substitute a positive constant, $\lambda^2 > 0$, for $\lambda(t)$ in Eq. (40a) to yield

$$\frac{d}{dt}[\Phi_j(t)] + \lambda^2\Phi_j(t) = \frac{j}{N}\lambda^2 \ , \ j = 1,2,...,N-1 \ . \tag{41}$$

Now, not only are solutions to Eq. (41) stable, but λ^2 can be chosen to adjust the decay rate of a

perturbation to its equidistributed position. This idea is similar to one proposed by Hyman (cf., Coyle, Flaherty, and Ludwig (ref 38)). Notice that unlike the neutrally stable case (cf., Eq. (38)), an initial perturbation of Φ_j, $j = 1,2,...,N-1$, decaying to zero does imply that the associated initial mesh perturbation of x_j, $j = 1,2,...,N-1$, decays to zero.

Example 6

Reconsider Example 4 where $w(x,t)$ was given by Eq. (26). Recall that Eq. (32) generated neutrally stable mesh motion because $\bar{L}(t) = 1$. Solutions of Eq. (41) should asymptotically approach the equidistributed positions. In Figure 6 (at the end of this section), meshes produced by both Eqs. (31) (dashed curves) and (41) (solid curves) are displayed. As predicted, mesh trajectories generated by Eq. (41) approach those generated by Eq. (31) as time progresses. As in Example 4, Simpson's rule with $M = 200$ was used to evaluate all integrals, a mesh of $N = 10$ elements was equidistributed, and an initial perturbation of $\delta x_j(0) = 0.025$, $j = 1,2,...,N-1$, was introduced. A value of $\lambda^2 = 1$ was used, and Eq. (41) was solved using a version of the differential-algebraic solver, DASSL (cf., Petzold (ref 37)).

Example 7

Reconsider Example 5 where $w(x,t)$ was given by Eq. (29). Recall that Eq. (38) generated neutrally stable mesh motion. Solutions of Eq. (41) should asymptotically approach the equidistributed position. In Figure 7 (at the end of this section), meshes produced by both Eqs. (31) (dashed curves) and (41) (solid curves) are displayed. As predicted, mesh trajectories generated by Eq. (41) approach those generated by Eq. (31) as time progresses. As in Example 5, Simpson's rule with $M = 200$ was used to evaluate all integrals, a mesh of $N = 10$ elements was equidistributed, and an initial perturbation of $\delta x_j(0) = 0.025$, $j = 1,2,...,N-1$, was introduced. A value of $\lambda^2 = 1$ was used, and Eq. (41) was solved using a version of the differential algebraic solver DASSL (cf., Petzold (ref 37)).

Another positive feature of these schemes is that extending them to higher dimensions is easily accomplished with all of their stability properties left intact. For simplicity, consider a rectangular two-dimensional domain

$$\Omega = \{(x,y) \,|\, a \le x \le b \,,\, c \le y \le d\} \tag{42}$$

and the extension of Eq. (38) to Ω. To that end, define

$$\Psi(x,y,t) = \frac{\int_a^x \int_c^y w(\zeta,\eta,t)\,d\eta\,d\zeta}{\int_a^b \int_c^d w(\zeta,\eta,t)\,d\eta\,d\zeta} \tag{43}$$

where $w(x,y,t)$ is a positive weight function on Ω such that $\Psi(x,y,t)$ is a well-defined function with the necessary continuity properties. Furthermore, let

$$\Pi^2(t) = \{(x_j(t),y_k(t))\}\ ,\ j = 0,1,\ldots,N_x\ ,\ k = 0,1,\ldots,N_y\ . \tag{44a}$$

denote a partition of Ω into $N_x \times N_y$ subrectangles at any time t such that

$$a = x_0(t) < x_1(t) < \ldots < x_{N_x}(t) = b\ , \tag{44b}$$

$$c = y_0(t) < y_1(t) < y_{N_y}(t) = d\ . \tag{44c}$$

In order for $\Pi^2(t)$ to move in a neutrally stable manner for any initial partition $\Pi^2(0)$, demand that it obey the following equations for $t > 0$:

$$\frac{d}{dt}[\Psi(x_j(t),d,t)] = 0\ ,\ j = 1,2,\ldots,N_x-1\ , \tag{45a}$$

$$\frac{d}{dt}[\Psi(b,y_k(t),t)] = 0\ ,\ j = 1,2,\ldots,N_y-1\ . \tag{45b}$$

Note that the stability of the two-dimensional movement is guaranteed by the one-dimensional theory since Eq. (45a) is equivalent to one-dimensional movement in the x-direction, while Eq. (45b) is equivalent to one-dimensional movement in the y-direction.

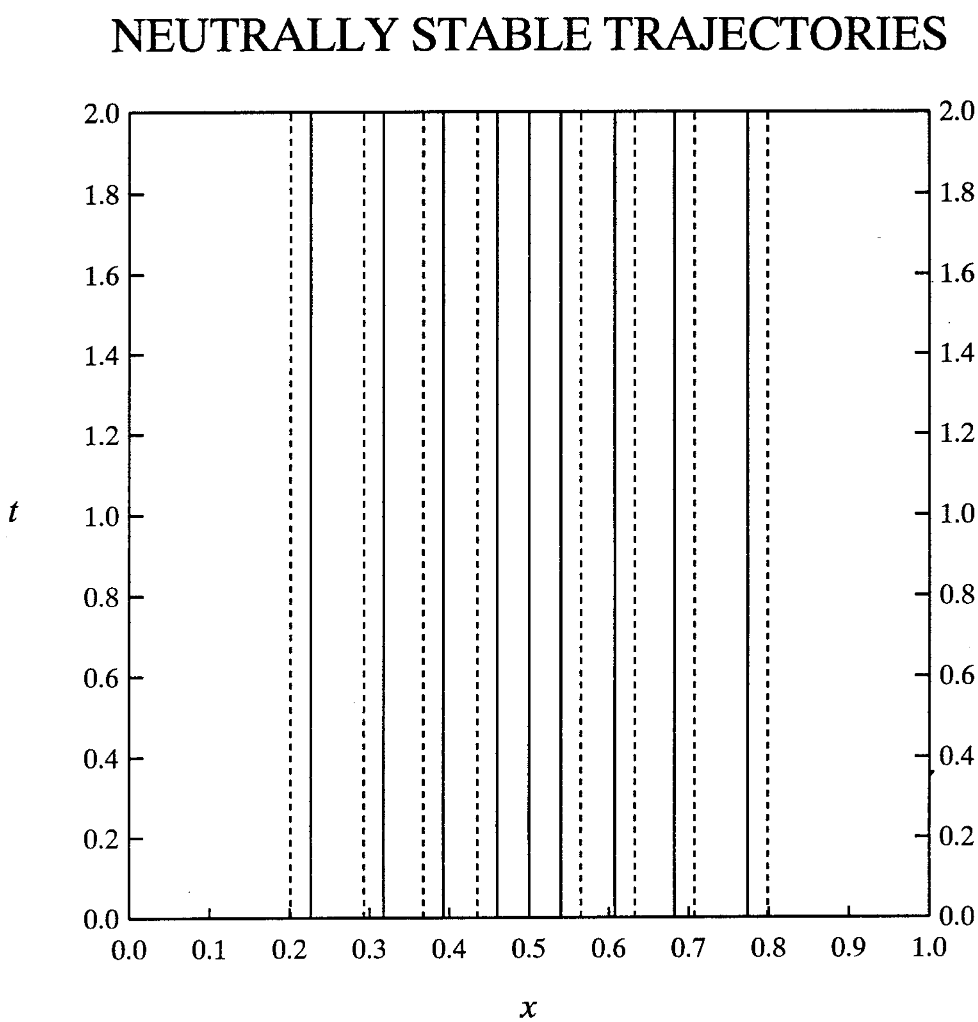

Figure 4. Mesh trajectories for Example 4.

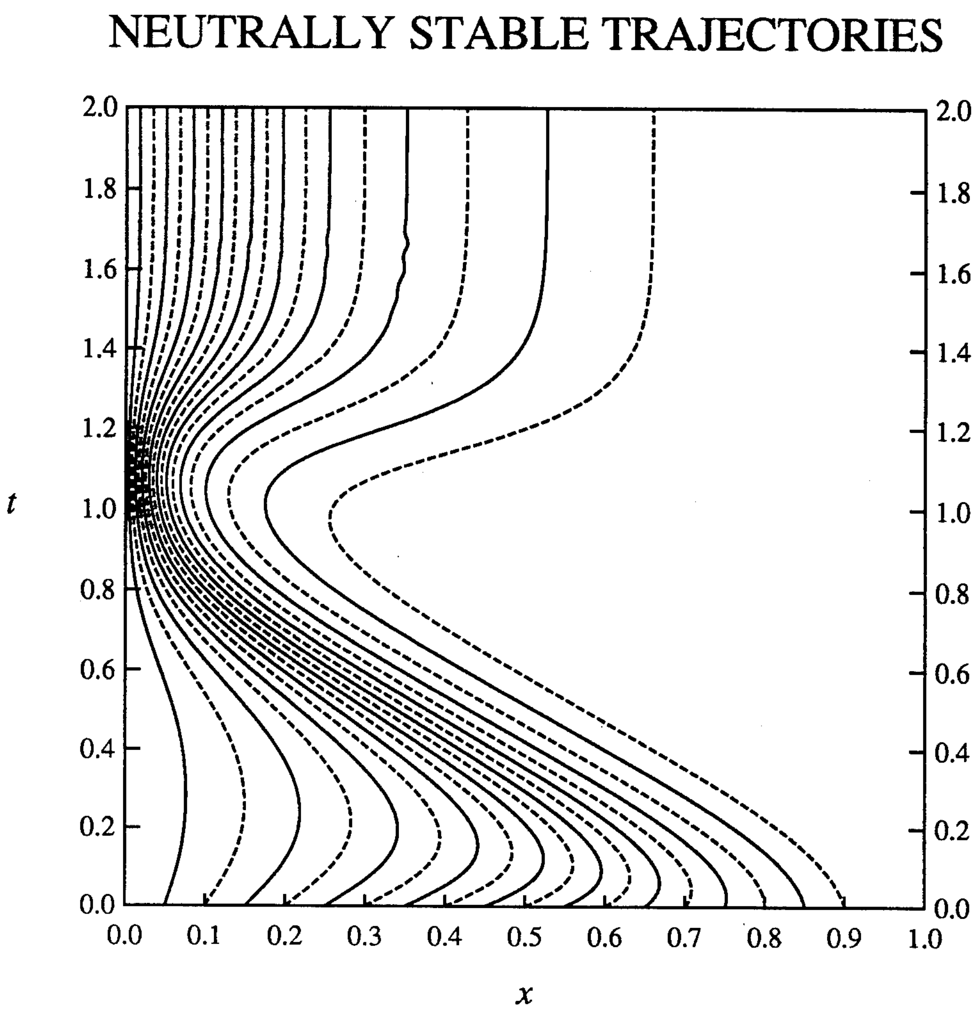

Figure 5. Mesh trajectories for Example 5.

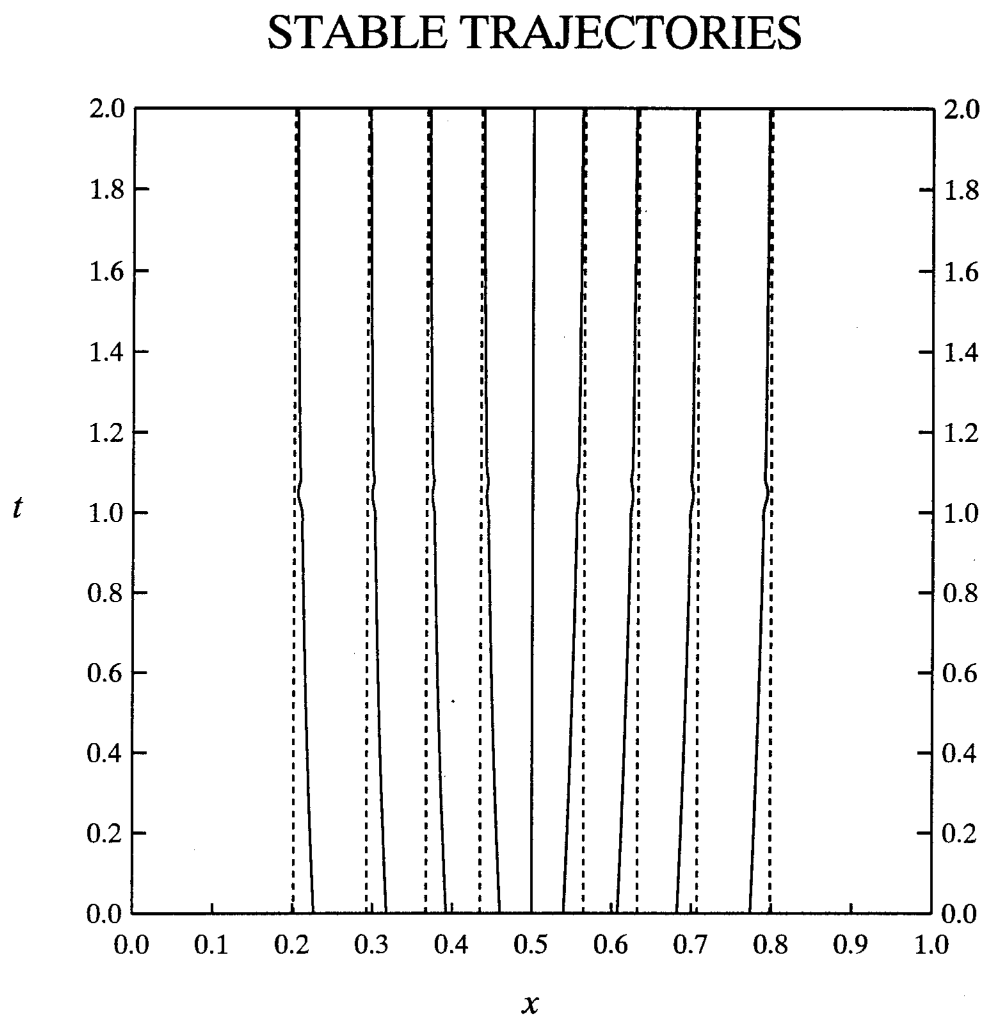

Figure 6. Mesh trajectories for Example 6.

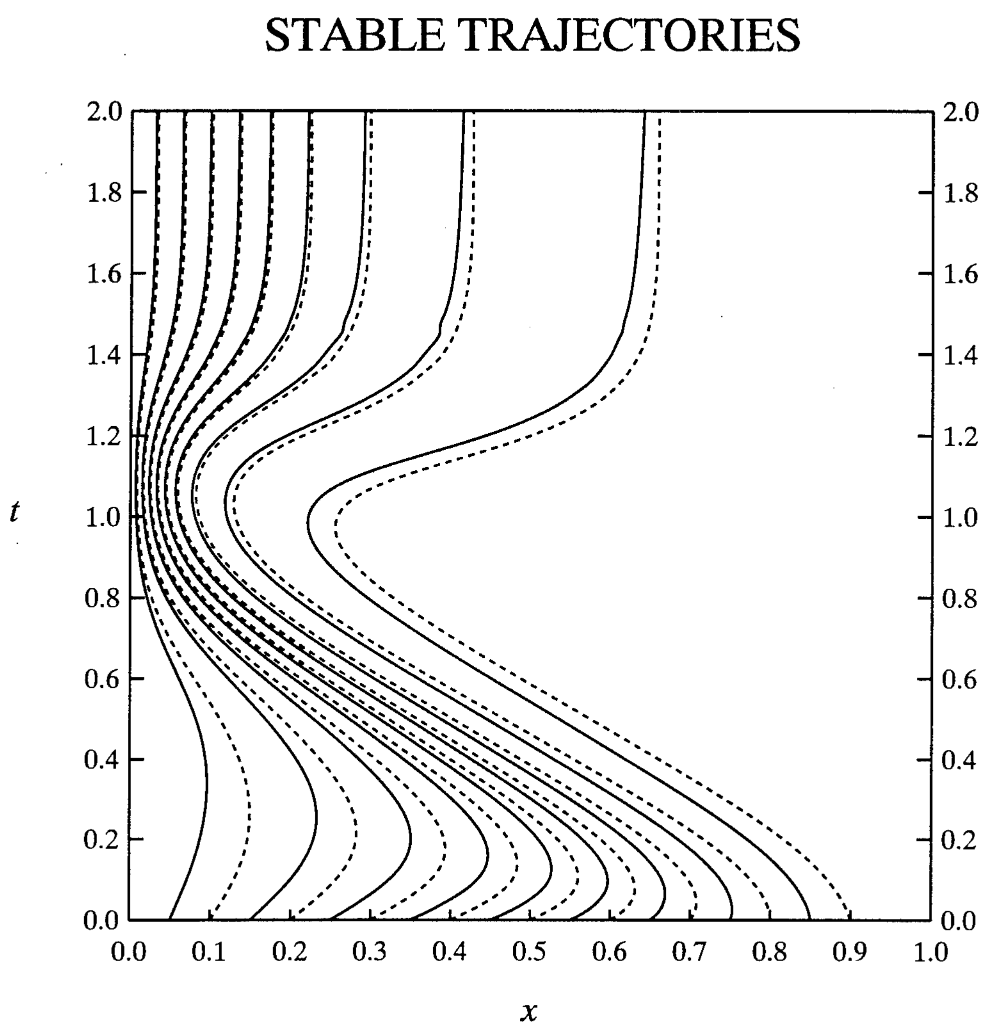

Figure 7. Mesh trajectories for Example 7.

MESH MOVEMENT IMPLEMENTATION

Recall that the purpose of investigating mesh moving schemes was to develop an effective tool to aid in the process of solving PDEs numerically. In the Mesh Dynamics: Linear Stability and Mesh Dynamics: Neutral Stability sections, the stability of mesh movement was discussed in isolation from its use with a PDE solver. The reason was that if mesh movement is not stable, then there would be no hope of it being a useful numerical tool. Now that the stability question has been answered, the question of implementation in a PDE solver needs to be addressed.

The first consideration is the choice of a mesh moving scheme. Since an unstable scheme is not an option, the choice would seem to be between a neutrally stable scheme (cf., Eq. (38)) or an asymptotically stable one (cf., Eq. (41)).

Usually in the field of numerical analysis, asymptotically stable schemes are preferred (cf., e.g., Lapidus and Pinder (ref 39) and Richtmyer and Morton (ref 40)). This is because computational errors are unavoidable, and asymptotically stable methods are best at minimizing the consequences of those errors. However, in this instance, the choice of a mesh moving scheme should be more related to the nature of the associated PDE solver.

If the solver is topologically invariant, i.e., mesh refinement is not present (cf., Davis and Flaherty (ref 14) and Miller and Miller (refs 20,21)), then an asymptotically stable mesh moving scheme is indeed the method of choice. Since the dimension of the mesh is fixed, the best one can do is position them optimally. This is precisely the situation where an asymptotically stable scheme works best.

However, if, as is proposed here, refinement will be performed in conjunction with mesh movement, then a neutrally stable scheme is preferred. This is because a neutrally stable scheme is independent of the number of mesh points (cf., Eq. (38)). Also, there is no unknown parameter λ to choose.

Suppose, for example, that refinement demands a new point, $x^n_{j+1/2}$, to be added at time t^n between existing points x^n_j and x^{n+1}_j. To determine how $x_{j+1/2}(t)$ should move for $t > t^n$, simply solve the following initial value problem:

$$\frac{d}{dt}[\Phi_{j+1/2}(t)] = \frac{d}{dt}[\Phi(x_{j+1/2}(t),t)] = 0 \ , \ t > t^n \ , \tag{46a}$$

$$\Phi_{j+1/2}(t^n) = \frac{\int_a^{x^n_{j+1/2}} w(\zeta,t)\,d\zeta}{\int_a^b w(\zeta,t)\,d\zeta} \ . \tag{46b}$$

If, on the other hand, refinement requires deletion of a point, then mesh motion continues with the remaining points moving according to Eq. (38).

In this way, theoretically, when assuming exact integration, the addition or deletion of points via refinement has no effect on the movement of any previously existing points that remain after refinement. The movement of new points will begin at the instant of their creation and will be unaffected by anything the previously existing points have been or will be doing. As a consequence, we chose to implement the neutrally stable scheme Eq. (38) over the asymptotically stable one.

The next consideration is the choice of the equidistribution function $w(x,t)$ (cf., Eq. (30)). This choice should be related to the reasons for incorporating mesh movement into the PDE solver since $w(x,t)$ will determine the qualitative nature of the movement (cf., Eq. (38) or (41)).

In general, the aim of any adaptive strategy is to increase the reliability and reduce the temporal and spatial complexity of the solution procedure. With h-refinement, this takes the form of solving a problem to some specified accuracy using a coarser discretization level than would be necessary without adaptivity.

There seems to be no general consensus, however, as to what $w(x,t)$ should be in order to simplify the solution process. Some researchers, for example, choose $w(x,t)$ to be proportional to some physical quantity of interest and/or proportional to some derivative of the solution (cf., Bell and Shubin (ref 13), Davis and Flaherty (ref 14), Dorfi and Drury (ref 15), Dwyer (ref 16), Rai and Anderson (ref 23), Russell and Ren (ref 24), Smooke and Koszykowski (ref 26), Verwer, Blom, Furzeland, and Zegeling (ref 28), and White (ref 29)). Still others attempt to relate $w(x,t)$ to the residual error (cf., Miller and Miller (refs 20,21)) or the local discretization error (cf., Adjerid and Flaherty (ref 1)). The underlying assumption with any choice is that reasonable approximations to the chosen monitors exist.

When error estimates are available (cf., Adjerid and Flaherty (ref 1)), it would seem appropriate to let these estimates control the movement. However, more often than not, these estimates lead to erratic mesh motion due to their dependency on mesh location. Some researchers reduce this difficulty by coupling the error estimation and mesh moving process with the PDE solution (cf., Adjerid and Flaherty (ref 1)).

Experience has shown that the estimates developed for use in AFEM (cf., Coyle and Flaherty (ref 30)) do not produce reliable mesh motion, when left uncoupled from the solution process. However, our desire is to develop a mesh moving strategy that is separate from the PDE solver, not because coupling is ineffective (cf., Adjerid and Flaherty (ref 1)), but rather because of the greater flexibility provided by an uncoupled approach to mesh moving. In this way, movement can be simple to implement, easily invoked or ignored during the solution process, transparently combined with a variety of PDE solvers which have no mesh movement capabilities, and extensible to higher dimensional problems.

When error estimates are unavailable or inappropriate, picking $w(x,t)$ to be proportional to some combination of the approximate solution and/or some of its derivatives seems plausible. This is because the discretization error of any PDE solver can usually be expressed in terms of some solution derivatives (cf., e.g., Lapidus and Pinder (ref 39), Richtmyer and Morton (ref 40), and Strang and Fix (ref 41)).

At first, we proceeded along lines similar to Davis and Flaherty (ref 14), and chose w to be proportional to the second spatial derivative of the approximate solution. The spatial error of a piecewise linear approximation is proportional to the corresponding exact spatial derivative so equidistributing such a w should reduce the spatial error component of the method. However, when left uncoupled from the solution, w must be determined at an advanced time level from past data in order to propagate the mesh to that advanced time level. Experiments showed that although this strategy was successful for the first few time steps, numerical errors accumulated to the point where the extrapolation of this w would produce highly inaccurate approximations to the second spatial derivative and, hence, unreliable mesh motion.

Experiments using the exact second spatial derivative for problems where the exact solution was known proved revealing. Although the movement did reduce the spatial error component, the temporal error component of the method increased to the point where the total error actually increased as well. This was unacceptable. As a result, we began to investigate choices for w that addressed temporal as opposed to spatial concerns (cf., e.g., Ewing, Russell, and Wheeler (ref 17), Hyman (ref 18), Kansa, Morgan, and Morris (ref 19), and Petzold (ref 22)). This also had the appeal of simplifying the extension to higher dimensions because only the spatial dimensions increase and the nature of the temporal dimension remains the same.

Choosing w to be proportional to first and/or second temporal derivatives of the approximate solution proved unsatisfactory. Again, experiments indicated that extrapolation would eventually produce inaccurate approximations to these temporal derivatives.

Experimentation with exact temporal derivatives was successful, however. The temporal component of the error decreased and the spatial component did not increase significantly, so the total error also decreased as a result of the movement (cf., Coyle (ref 42)).

Only when extrapolating the approximate solution to advanced time levels were numerical errors small enough so as not to degrade the approximation significantly. This is because the approximate solution is known to a higher order of accuracy than its derivatives.

At first, choosing w to be proportional to the approximate solution did not seem so appealing since discretization errors are more closely related to derivatives of solutions. However, other researchers have had success when moving the mesh so that the variation in time of the solution is reduced in the transformed coordinates (cf., e.g., Ewing, Russell, and Wheeler (ref 17), Hyman (ref 18), Kansa, Morgan, and Morris (ref 19), and Petzold (ref 22)). This seems plausible since a slowly varying solution implies small temporal derivatives.

Upon reexamining Eq. (38), one sees that in the transformed coordinates, the quantities $\Phi_j(t), j = 1,2,...,N-1,$ are demanded to remain constant not just slowly varying. Such a scheme, with w chosen to be proportional to the approximate solution, should also keep temporal derivatives small, and, hence, temporal errors, as experimentation has testified (cf., Coyle and Flaherty (ref 32)). In addition, when considering the extension to higher dimensions, no extra derivatives enter the computation.

Our decision has been to let $w(x,t)$ be proportional to the L_2 norm of the approximate solution. Since Eq. (38) simply states to keep $\Phi_j(t), j = 1,2,...,N-1,$ constant from time step to time step, the following procedure is performed. First, linearly extrapolate the mesh to time

level t^{n+1} from mesh positions at time levels t^n and t^{n-1}. If mesh trajectories cross or leave the domain, then delete these offending points. This first mesh is not intended to be the computational mesh but rather a mesh on which to determine the extrapolated values of $w(x,t^{n+1})$. As such, nothing sophisticated is performed to avoid possible mesh instabilities.

Next, linearly extrapolate the approximate solution onto the mesh at time level t^{n+1} from data at time levels t^n and t^{n-1}. Then determine $w(x,t^{n+1})$ as the L_2 norm of this extrapolated solution.

Finally, the new mesh points $\{x_j^{n+1}\}_{j=1}^{N-1}$ at time level t^{n+1} are determined such that

$$\Phi_j(t^{n+1}) = \Phi_j(t^n) \ , \ j = 1, 2, \dots , N-1 \ . \tag{47}$$

Eq. (47) is solved by the method detailed in the Static Spatial Equidistribution section.

SUMMARY

An extension of one-dimensional, static mesh equidistribution to a time-dependent domain was proposed. The purpose of this extension was to provide aid in the process of solving partial differential equations numerically.

The stability of this extension was examined. As a result, we explained why many intuitively obvious schemes for calculating equidistributing meshes for time-dependent partial differential equations are unstable. In particular, we derived a stability condition on the equidistribution density $w(x,t)$ that can easily be verified in practice. In addition, we constructed both neutrally stable and asymptotically stable mesh moving techniques as demonstrated by the various examples of the Mesh Dynamics: Neutral Stability section, as well as proposed an extension to higher dimensional domains. The neutrally stable scheme was incorporated into a numerical method for solving PDEs that already possessed error estimation and mesh refinement capabilities.

The results of this report indicate that mesh movement is still a credible adaptive option. The problems researchers have experienced with mesh moving are not because of any intrinsic failure of the approach, but rather, are a result of a lack of understanding of the stability properties of the process. This led to the stability analyses of Mesh Dynamics: Linear Stability and Mesh Dynamics: Neutral Stability sections as well as to the construction of stable moving schemes.

Mesh movement cannot guarantee that a computed solution is accurate to some prescribed tolerance, however, because the discretization level is fixed. In order to overcome this obstacle, a local mesh refinement algorithm with error estimation capabilities has also been incorporated into AFEM. Local mesh refinement schemes can be costly, due to the necessity of recomputing the solution; however, proper mesh motion should permit as few levels of refinement as possible (cf., Coyle and Flaherty (ref 32)).

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